



Dear CEMBIO members,

It has been a tough semester, so tough that we couldn't even find the time to produce our quarterly newsletter. Under the influence of the pandemic, time seems a continuous 18 months long; however, in between we have had Filomena, but also very good news: two promotions in the group: Antonia García to Full Professor and Javier Rupérez to Lecturer, and a new Ph.D. graduated with honors: Miguel Fernández. CONGRATULATIONS!! As you can see below, despite the difficulties, the year has been very productive.

We miss our day out which is a good excuse to enjoy and share time out of the office, but I do hope that next year we will be able to have more celebrations altogether.

Coral

## Spotlight

The new Agilent 6546 LC/Q-TOF equipment arrived in June and is fully functional! Accurate Mass Spectrometry SAI at USP-CEU is ready

Prof. Coral Barbas

En esta clasificación de investigadores se ha incluido también a **Coral Barbas** que dirige el Centro de Excelencia en Metabolómica y Bioanálisis (CEMBIO), y la Escuela Internacional de Doctorado CEINDO, que aúna a las tres universidades CEU. Coral Barbas es doctora *Honoris Causa* en la Universidad Médica de Białystok (Polonia) y Premio de la Sociedad Belga de Ciencias Farmacéuticas. Su área de investigación se centra en el bioanálisis con el desarrollo de metodologías analíticas para estudios biológicos y la Metabolómica aplicada a búsqueda de marcadores diagnósticos, pronósticos o del efecto de un tratamiento mediante espectrometría de masas.



Stanford University



## Events Activities & Seminars

March 12 2021 | Lipidomics update: Unveiling the new rules of the game. by **Carolina González Riaño**

June 25 2021 | Online training on Agilent data processing for GC-MS and LC-MS analysis to researchers from Steno Diabetes Center Copenhagen by **Carolina González Riaño** and **Alma Villaseñor**

April 8 2021 | Seminar about Analysis of variance – simultaneous component analysis (ASCA or ANOVA-SCA) by **Santiago Angulo**

## Conferences



17<sup>th</sup> Annual Conference of the Metabolomics Society  
**METABOLOMICS2021**  
JUNE 22-24 ONLINE

June 22-24 2021 | 17<sup>th</sup> Annual Conference of the Metabolomics Society

- **Poster Presentation:** Metabolomic reprogramming of C57BL/6-macrophages during early infection with *L. amazonensis*. **Maricruz Mamani-Huanca, Coral Barbas, Angeles López-González and others.**
- **Poster Presentation:** Aspergillus Metabolome Database (AMDB) for Mass Spectrometry Metabolomics. **Alberto Gil-de-la-Fuente, Maricruz Mamani-Huanca, Coral Barbas, Abraham Otero and others.**
- **Poster Presentation:** Metabolomics analysis of serum from patients with anaphylactic reactions from different mechanisms. **David Obeso, Alma Villaseñor, Coral Barbas and others.**
- **Poster Presentation:** Metabolomics of feces reveal differences between infants, their mothers, and their grandmothers in metabolites from microbiota-host co-metabolism. **Tomás Barker-Tejeda, Elisa Zubeldia-Varela, David Rojo, Fernanda Rey-Stolle, Alma Villaseñor, Coral Barbas and others.**
- **Poster Presentation:** Exploring prognostic biomarkers of early prodromal Parkinson's disease in the Spanish EPIC cohort through a multiplatform metabolomics approach. **Carolina González-Riaño, Jorge Saiz, Coral Barbas and others.**
- **Poster Presentation:** The metabolic changes behind the improvement of cognitive functions induced through probiotic supplementation in patients with major depressive disorder. **Joanna Godzien, Cecilia Barbas, Antonia García, Coral Barbas and others.**
- **Poster Presentation:** COVID-19 plasma samples analysis by CE MS as a snapshot for metabolic alterations. **Olhane Albóniga, Coral Barbas and others.**
- **Poster Presentation:** Alterations of modified amino acids patterns in chronic kidney disease (CKD). **Paula Cuevas-Delgado, Coral Barbas and others.**
- **Poster Presentation:** Ceramide composition in exosomes for characterization of glioblastoma stem-like cell phenotypes. **Raquel Melero-Fernández de Mera, Alma Villaseñor, David Rojo, Ana Gradillas, Coral Barbas and others.**

July 10-12 2021 | EAACI Hybrid Annual Congress

- **Oral presentation:** Metabolic changes in the prediction of severe anaphylactic reactions. **Alma Villaseñor, David Obeso, Coral Barbas and others.**
- **Oral presentation:** Olive allergic patients non responders to AIT present specific immune and metabolic profile before treatment. **Juan Rodríguez-Coira, Alma Villaseñor, David Obeso and others.**
- **Poster Presentation:** Molecular mechanisms of anaphylaxis characterized by metabolomics. **David Obeso, Alma Villaseñor and others.**
- **Poster Presentation:** Metabolomics: a novel approach in the study of cow's milk allergy. **Tomás Barker-Tejeda, Elisa Zubeldia-Varela, David Rojo, Fernanda Rey-Stolle, Coral Barbas and others.**
- **Poster Presentation:** Biological interpretation of the metabolic alterations detected in a murine model of allergic enteritis. **Elisa Zubeldia-Varela, Tomás Barker-Tejeda, David Rojo, Alma Villaseñor, Coral Barbas and others.**
- **Poster Presentation:** Understanding the role of allergy in the systemic and local inflammation induced by nasal polyps. **M<sup>a</sup> Isabel Delgado-Dolset, David Obeso, Coral Barbas, Alma Villaseñor and others.**



July 12-15, 2021 | 37<sup>th</sup> International Symposium on Microscale Separations and Bioanalysis (e-MSB2021)

- **Poster Presentation:** From (Almost) Nothing To (Almost) Everything: Metabolic Phenotyping Of Developing Mice Hearts. **Carolina González-Riaño, Coral Barbas and Javier Rupérez.**



June 30-July 3, 2021 | 15<sup>th</sup> World Immune Regulation Meeting

- **Oral Presentation:** T cells of non-responders to AIT present distinctive metabolic profile before treatment and is linked to their inflammatory profile. **Juan Rodríguez-Coira, Alma Villaseñor, C. Gómez-Casado, J. Sánchez-Solares, David Obeso and others.**



## Publications

Evaluation of the Cytotoxicity of Ayahuasca Beverages

Simão A. Y., Gonçalves J., Gradillas A., García A., Restolho J., Fernández N., Rodilla J. M., Barroso M., Duarte A. P., Cristóvão A. C., Gollardo E.

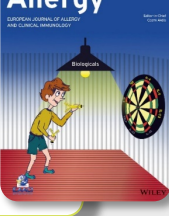
*Molecules*, March 2021 DOI: [10.3390/molecules25235594](https://doi.org/10.3390/molecules25235594)



SARS-CoV-2 candidate vaccines - composition mechanisms of action and stages of clinical development

Rodríguez-Coira J., Sokolowska M.

*Allergy*, December 2020 DOI: [10.1111/all.14714](https://doi.org/10.1111/all.14714)



Renal tubule Cpt1a overexpression protects from kidney fibrosis by restoring mitochondrial homeostasis

Miguel V., Tituaña J., Herrero J., Herrero L., Serra D., Cuevas P., Barbas C., et al.

*J. Clin. Invest.*, January 2021 DOI: [10.1101/2020.02.18.952440](https://doi.org/10.1101/2020.02.18.952440)



Uncovering the influence of diet and gut microbiota in human serum metabolome

Obeso D., Zubeldia-Varela E., Villaseñor A.

*Allergy*, February 2021 DOI: [10.1111/all.14770](https://doi.org/10.1111/all.14770)



Extracellular and intracellular zilpaterol and clenbuterol quantification in Hep G2 liver cells by UPLC-PDA and UPLC-MS/MS

Piña-Olmos S., Dolores-Hernández M., Villaseñor A., et al.

*J. Pharm. Biomed. Anal.*, February 2021 DOI: [10.1016/j.jpba.2020.113817](https://doi.org/10.1016/j.jpba.2020.113817)



Combined Genome, Transcriptome and Metabolome Analysis in the Diagnosis of Childhood Cerebellar Ataxia

Ching-López A., Martínez-González L.J., Arabal L., Sáiz J., Gavilán Á., Barbas C., et al.

*Int. J. Mol. Sci.*, March 2021 DOI: [10.3390/ijms22062990](https://doi.org/10.3390/ijms22062990)



Aspergillus Metabolome Database for Mass Spectrometry Metabolomics

Gil-de-la-Fuente A., Mamani-Huanca M., Stroe M.C., Saugar S., García-Alvarez A., Brakhage A.A., Barbas C., Otero A.

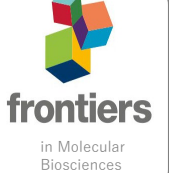
*J. Fungi*, May 2021 DOI: [10.3390/jf7050387](https://doi.org/10.3390/jf7050387)



Understanding Systemic and Local Inflammation Induced by Nasal Polyposis: Role of the Allergic Phenotype

Delgado-Dolset M. I., David O., Sánchez-Solares J., Mera-Berriatua L., Fernández P., Barbas C., Fresnillo M., Chivato T., Barber D., Escobedo M., Villaseñor A.

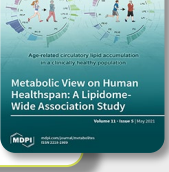
*Front. Mol. Biosci.*, May 2021 DOI: [10.3389/fmolb.2021.662792](https://doi.org/10.3389/fmolb.2021.662792)



Metabolomics in the Identification of Biomarkers of Asthma

Villaseñor A., Eguiluz-García I., Moreira A., Wheelock C.E., Escobedo M.M.

*Metabolites*, May 2021 DOI: [10.3390/metabo11060346](https://doi.org/10.3390/metabo11060346)



In vitro generation of oxidized standards for lipidomics. Application to major membrane lipid components

Barker-Tejeda T. C., Villaseñor A., González-Riano C., López López A., Gradillas A., Barbas C.

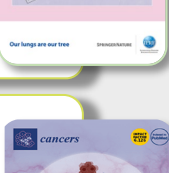
*J. Chromatogr. A*, May 2021 DOI: [10.1016/j.chroma.2021.462254](https://doi.org/10.1016/j.chroma.2021.462254)



Noninvasive monitoring of evolving urinary metabolic patterns in neonatal encephalopathy

Piñero-Ramos J.D., Cascant M.M., Núñez-Ramiro A., López-González Á., Salazar-García Á., Albach-Delgado A., Martínez-Rodilla J., Llorens-Salvador R., Sanjuan-Herrero D., Quintás G., Barbas C., et al.

*Pediatr. Res.*, May 2021 DOI: [10.1038/s41393-021-01553-z](https://doi.org/10.1038/s41393-021-01553-z)



Comprehensive Plasma Metabolomic Profile of Patients with Advanced Neuroendocrine Tumors (NETs). Diagnostic and Biological Relevance

Soldevilla, B., López-López, A., Lens-Pardo, A., Carretero-Puche, C., López-González, A., La Salvia, A., Gil-Calderon, B., Riesco-Martínez, M.C., Espinosa-Olarte, P., Sarmentero, J., Rubio-Cuesta, B., Rincón, R., Barbas, C., et al.

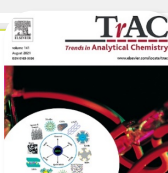
*Cancers*, May 2021 DOI: [10.3390/cancers13112634](https://doi.org/10.3390/cancers13112634)



Analytical Approaches for studying Oxygenated Lipids in the search of Potential Biomarkers by LC-MS

Villaseñor A., Godzien J., Barker-Tejeda T. C., González-Riano C., López-López A., Dudzik D., Gradillas A., Barbas C.

*TrAC. Trends Anal. Chem.*, June 2021 DOI: [10.1016/j.trac.2021.116367](https://doi.org/10.1016/j.trac.2021.116367)



Metabolomics reveals synergy between Ag and g-C3N4 in Ag/g-C3N4 composite photocatalysts: a unique feature among Ag-doped biocidal materials

Kubacka, A., Rojo, D., Muñoz-Batista, M.J., Barbas C., et al.

*Metabolomics*, June 2021 DOI: [10.1007/s11306-021-01804-4](https://doi.org/10.1007/s11306-021-01804-4)



Metabolomic Reprogramming of C57BL/6-Macrophages during Early Infection with *L. amazonensis*

Mamani-Huanca M., Muxel S.M., Acuña S.M., Floeter-Winter L.M., Barbas C., López-González A.

*Int. J. Mol. Sci.*, June 2021 DOI: [10.3390/ijms22136883](https://doi.org/10.3390/ijms22136883)



A Preliminary Study Showing the Impact of Genetic and Dietary Factors on GC-MS-Based Plasma Metabolome of Patients with and without PROX1-Genetic Predisposition to T2DM up to 5 Years Prior to Prediabetes Appearance

Mojak, P., Miniewska, K., Godlewski, A., Adamska-Patrano, E., Samczuk, P., Rey-Stolle, F., Bauer, W., Barbas, C., et al.

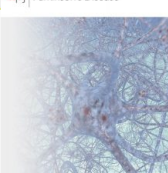
*Curr. Issues Mol. Biol.*, June 2021 DOI: [10.3390/cimb43020039](https://doi.org/10.3390/cimb43020039)



Searching for prognostic biomarkers of Parkinson's Disease development in the Spanish EPIC cohort through a multiplatform metabolomics approach

Carolina González-Riaño, Jorge Saiz, Coral Barbas, et al.

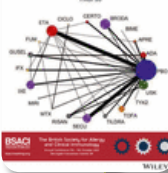
*NPJ Parkinson's Dis.*, July 2021 DOI: [10.1101/2021.03.02.21252744](https://doi.org/10.1101/2021.03.02.21252744)



Characterization of anaphylaxis reveals different metabolic changes depending on severity and triggers

Perales-Chorda C., Obeso D., Twomey L., Rojas-Benedicto A., Puchades-Carrasco L., Roca M., Pineda-Lucena A., Laguna J. L., Barbas C., Esteban V., Martí-Garrido J., Ibañez-Echevarría E., López-Salgueiro R., Barber D., Villaseñor A., et al.

*Clin. Exp. Allergy*, July 2021 DOI: [10.1111/cea.13991](https://doi.org/10.1111/cea.13991)



The Role of Sphingolipids in Allergic Disorders

Díaz-Perales A., Escobedo M.M., Garrido-Arandia M., Obeso D., et al.

*Front. Allergy*, July 2021 DOI: [10.3389/falgy.2021.675557](https://doi.org/10.3389/falgy.2021.675557)



The importance of metabolism for immune homeostasis in allergic diseases

Rodríguez-Coira J., Villaseñor A., Izquierdo E., Huang H., Barker-Tejeda T.C., et al.

*Front. Immunol.*, July 2021 DOI: [10.3389/fimmu.2021.692004](https://doi.org/10.3389/fimmu.2021.692004)



Comparative metabolomics analysis of bronchial epithelium during barrier establishment after allergen exposure

López-Rodríguez J.C., Rodríguez-Coira J., Benedité S., Barbas C., Barber D., Villalba M., Escobedo M.M., Villaseñor A., et al.

*Clin. Transl. Allergy*, July 2021



EAACI Global Atlas of Asthma 2021 Update

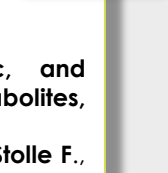
CHAPTER 8: Omics  
Escobedo M., Boerentaller K., Villaseñor A., et al.

EAACI the European Academy of Allergy and Clinical Immunology  
<https://www.eaaci.org/newsfeed/newsfeed-bottom/4790-globalatlasofasthma>



Parasite Genomics

Part of the Methods in Molecular Biology series. (NM, volume 2369)  
July 2021 DOI: [10.1007/978-1-0716-1681-9](https://doi.org/10.1007/978-1-0716-1681-9)



CHAPTER 12: Integration of Genomic and Transcriptomic Data to Elucidate Molecular Processes in Babesia divergens

González L.M., Sevilla E., Fernández-García M., et al.

CHAPTER 13: Integration of Functional Genomic, Transcriptomic, and Metabolomic Data to Identify Key Features in Genomic Expression, Metabolites, and Metabolic Pathways of Babesia divergens

Fernández-García M., Sánchez-Flores A., González L.M., Barbas C., Rey-Stolle F., Sevilla E., García A., Montero E.

## Spotlight

Promotion to:

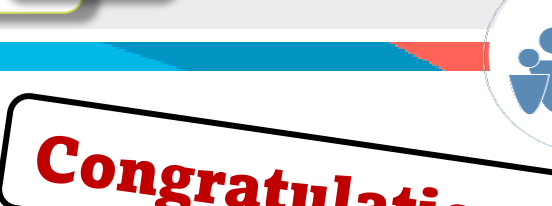
✓ **Miguel Fernández García**. PhD

July 1 2021 | "Development and Application of Multiplatform Metabolomic Pipelines for the Study of Infectious Diseases"

✓ **Antonia García**. Full professor of Analytical Chemistry (Catedrática)

✓ **Javier Rupérez**. Lecturer of Analytical Chemistry (Profesor Titular)

&: ✓ **David Rojo**. On the birth of his daughter!



## Members Corner



✓ **Carolina González-Riaño**

Press Note in ABC.

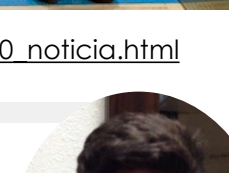
ABC FORMACIÓN

[https://www.abc.es/formacion/abci-investigacion-camino-mas-necesario-tambien-mas-intransitable-202105182120\\_noticia.html](https://www.abc.es/formacion/abci-investigacion-camino-mas-necesario-tambien-mas-intransitable-202105182120_noticia.html)



**EAACI Hybrid Congress 2021** 10-12 July

✓ **David Obeso Montero**



Press Note. "Molecular mechanisms of anaphylaxis characterized by metabolomics"

Has been selected as outstanding and suitable for a press release for the EAACI Hybrid Congress 2021

Farewell (not goodbye)

We would like to extend a warm farewell to our colleagues

Thank you for these years working together

We wish the very best for you on your upcoming journey and you know that our doors are always open for you!

✓ **Ángeles López López**

✓ **Marta López**



agencia española de medicamentos y productos sanitarios

## Research Mobilities - Outgoing

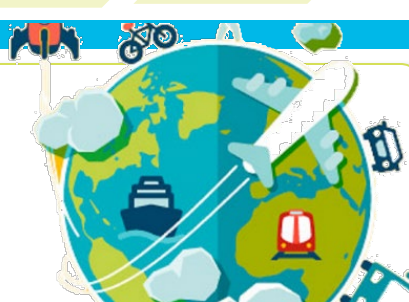
✓ **Maricruz Mamani**

➤ **March-July 2021** | Group of Molecular Nutrition and Metabolism (NUTRIMOL) CIAL-CSIC, Madrid.

✓ **Elisa Zubeldia**

➤ **January-April 2021** | Paul-Ehrlich-Institut, Langen, Germany.

Paul-Ehrlich-Institut



## Research Mobilities - Incoming

✓ **Bachelor final project:** **Carolina de Rosa** - University of Modena and Reggio Emilia, Italy. Erasmus program. Under the supervision of **Antonia García**

✓ **Ahsan Hameed**, PhD student in Białystok Medical University. Under the supervision of **Coral Barbas**

## Training Students

✓ **Master final project:** **Garazi González Sánchez**. Interuniversity Master in Drug Discovery. USP-CEU. Under the supervision of **Javier Rupérez**

✓ **Bachelor final project:** **Ana Sánchez Lorenzo**. Double Degree Pharmacy-Biotechnology. USP-CEU. Under the supervision of **Ana Gradillas** → with a CEU undergraduate research fellowship

✓ **Bachelor final project:** **Ana García García**. Degree in Biotechnology. UPM. Under the supervision of **Alma Villaseñor**

✓ **Bachelor final project:** **Gabriel Montero Tejedor**. Double Degree Pharmacy-Biotechnology. USP-CEU. Under the supervision of **Antonia García**

✓ **2<sup>nd</sup> year student:** **Patricia Muñoz Escudero**. Double Degree Pharmacy-Biotechnology. USP-CEU. Under the supervision of **Jorge Saiz**



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